General Information

Instructor: Prof. Joshua Schrier
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Meeting Time: by appointment

Prerequisites: Previous coursework in chemistry, physics, or computer science and consent of instructor.

Purpose: You are a scientist in training. This course is an opportunity to pursue a research project in the area of computational/theoretical chemistry in a tutorial-based fashion, to grow as a scientist. Scientists must be able to read the work of others, formulate interesting questions, address those questions (using their technical skills), and present their results to others. The deliverables listed below will serve as the evidence that you are growing in these skills.

Research Areas: Topics of interest this year include:
- Quantifying non-covalent interactions in organically template inorganic materials (e.g., organohalide perovskites and amine-templated vanadates); machine learning for chemical synthesis
- Machine learning for inorganic synthesis (“Dark reactions project”)—model development
- Simulation-based materials science research (e.g., silica bilayers, redox flow batteries)
- Orbital-specific valence calculations, applications to organometallic complexes.
- Deep learning approaches to electronic structure theory (specifically: approximate density matrix prediction)
- Web-development of a game for teaching organic spectroscopy

Grades: Grades will be calculated on the following basis: (see below)
- 20% Satisfying deliverables
- 20% Weekly progress slides
- 20% Demonstrating growth in independent problem solving (“ownership of project”) and in the six phases
- 20% Interim report (due end of Fall Semester)
- 20% Final report (due end of Spring Semester)

Deliverables: J-courses are awarded half a credit for enrollment over the entire year (both Fall and Spring semesters). You must enroll for the entire year to receive College credit. My expectations are that you will:
- Attend all weekly meetings, discussions.
- Spend at least 3 hours per week performing research
- Present progress slides at each weekly meeting. (see below)
- Demonstrate growth in the six phases of research (see below)
- Demonstrate growth in computational/numerical skills, e.g., through programming, use of unix operating system, use of software packages.
- Submit a short interim reports at the end of the fall semester, and a short final report at the end of the spring semester, explaining your research problem and the work that you performed.
Each week, please prepare two powerpoint-style slides, summarizing the following:

- **Slide 1:** What did you do last week? (What were the results? What were the problems/challenges?) What are you going to do next week?
- **Slide 2:** What did you read last week? What aspects are interesting/useful for your project?
  - Specifically: Relevant to your research project. These will typically be journal articles, but can also include technical tutorials or books. Pictures are valuable. These can include graphs of your results, key figures from journal articles, etc.

Be prepared to talk me through this during the first few minutes of our weekly meetings. These slides do not have to be particularly polished, but should convey your specific goals and outcomes. Note: These are a useful resource for preparing your interim and final reports.

**Six Phases:** Scientific research problems often involve the following phases.
1. Identifying the scientific problem
2. Creating a hypothesis
3. Developing specific aims
4. Identifying appropriate methods to perform the project
5. Interpreting data
6. Drawing conclusion

**Reports:** You are asked to submit short (2-3 pages is sufficient, but it can be longer if necessary) reports, describing your project at the end of the fall and spring semesters. Your reports should address the following questions:
1. What is the general problem, why is it interesting, and why is it hard? (1 paragraph)
2. What is your specific research question/problem? (1 paragraph)
3. Is there any relevant work on this question? Why is your approach better/novel? (1 paragraph)
4. What is your methodology/computational approach for solving this? (1-2 paragraphs)
5. What did you do? What did you learn? What problems/difficulties did you encounter, and how did you overcome them? (as long as you need)
6. What was the results? (1-2 paragraphs)

You are encouraged to include citations to the literature and figures that help support your claims. It goes without saying (but I’ll say it anyway) that this report should be well written and free from typographical and grammatical flaws.

**Honor Code:** In addition to the usual expectations about the “work being your own” and “avoiding plagiarism”, research has additional ethical requirements and challenges. To address this, one aspect of your project will be to learn about scientific research ethics. This is not only “a good idea”, but is also mandated as part of our federal research funding.

A series of online tutorials will serve as the initial component to your training
Go to the following link and create an account
After activating your account and logging on, please go to ‘Continue Tutorials’
You will be asked to join a group, select ‘Haverford College Sciences’ and work through the modules.
Please send me a PDF “printout” or screen snapshot of your completion.
We can discuss specific cases during the course of the academic year.
Learning Accommodations: Haverford College is committed to supporting the learning process for all students. Please contact me as soon as possible if you are having difficulties in the course. There are also many resources on campus available to you as a student, including the Office of Academic Resources (https://www.haverford.edu/oar/) and the Office of Access and Disability Services (https://www.haverford.edu/access-and-disability-services/). If you think you may need accommodations because of a disability, you should contact Access and Disability Services at hc-ads@haverford.edu. If you have already been approved to receive academic accommodations and would like to request accommodations in this course because of a disability, please meet with me privately at the beginning of the semester (ideally within the first two weeks) with your verification letter.
Oral Presentation:
The final week of class (27 Apr – 01 May) will be spent on short student presentations. For your chosen material you will discuss the “latest and greatest” results in synthesis and applications. If you are particularly interested in only one of these aspects, you may focus on that, or you may construct a more comprehensive survey of recent work for your material. Depending on enrollment, these will be 10-20 minutes long, and will be followed by questions from the audience. You are encouraged to use PowerPoint-type presentation software to enhance the effectiveness of your presentation.

Final Paper: Your goal is to compile a publication-quality mini-review article on the synthesis, properties, and applications of your material, which will be posted publicly for use by the broader scientific community. Your written and oral presentations, combined with the written and oral feedback you will have received from your classmates and I, will form a core of this work. In addition, it is intended that our time in class, and your peer-reviewing will stimulate you to explore new areas for your writing. Substantial revision of your working papers is strongly suggested!

Your final paper should be in the form of a “Perspectives” articles in Nano Letters or a review article in Chem. Rev. or Rev. Mod. Phys., and should be no more than 10000 words (about 20 pages) (excluding references and figures).

It will be extremely helpful if your citations include links to the papers (or at least DOI indicators to facilitate these links).

Please review “What Chemists Need to Know about Copyright”
http://pubs.acs.org/page/copyright/learning_module/index.html

The final papers are due by the end of finals period:
Seniors: Saturday 09 May at 5pm.
Others: Friday, 15 May at noon.
(Of course, you are welcome to turn it in earlier!)

The final paper is in lieu of a final examination.

Materials:
Lots of papers to summarize, need to be selective

Si, ZnO, Ge, TiO$_2$, GaN

GaAs, CdSe, CdS, ZnS, SnO2, InP, CdTe, InAs

InGaN, ZnSe, GaSb, Bi$_2$Te$_3$

Not as much work, can be more comprehensive about research progress